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ASSIMILATION OF BIO-OPTICAL PROPERTIES INTO COUPLED PHYSICAL, BIO-OPTICAL COASTAL MODEL

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ABSTRACT

Data assimilation experiments with the coupled physical, bio-optical model of Monterey Bay are presented. The approach is based on the representation of the error covariances in the subspace of the multivariate (bio-optical, physical) empirical orthogonal functions (EOFs) estimated from the model run. Estimated coupled bio-optical, physical error covariances are used in the Kalman gain update providing updates of coupled bio-optical properties in accord with the model dynamics and available observations. With the assimilation of satellite-derived bio-optical properties (chlorophyll-a and absorption due to phytoplankton), the model was able to reproduce intensity and tendencies in subsurface chlorophyll distributions observed at water samples locations in the Monterey Bay, CA. Data assimilation also improved agreement between the observed and model-predicted ratios between diatoms and small phytoplankton populations.

Keywords: Ocean data assimilation, Ecosystem dynamics, Ocean Modeling and Prediction, Coastal Processes, Interdisciplinary Oceanography

1. INTRODUCTION

The objective of this paper is to investigate whether the assimilation of satellite-derived bio-optical properties (as either chlorophyll-a or absorption coefficient) can improve the ecosystem model predictions of chlorophyll and phytoplankton population in a coastal ocean on time scales of 1-5 days. The specific time scale of 1 to 5 days is chosen because it is a time scale of availability of the atmospheric model forecast needed to force the oceanic model forecast. The atmospheric model forecast includes predictions of short-wave radiation (SWR), which is critical not only for forecasting the heat content and other physical properties of the ocean, but also for estimating the photosynthetically active radiation (PAR) which drives photosynthesis of the ecosystem model, and relevant to the forecast of the

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underwater light. Predictions of optical properties and underwater light are critical for numerous Navy operations, which rely on 1 to 5 days forecasts.

We designed our computational experiments to coincide with a large bio-optical field campaign that was conducted in Monterey Bay in June, 2008. The experiment was a collaboration between the NRL "Bio-Optical Studies of Predictability and Assimilation for the Coastal Environment (BIOSPACE)" project, Multidisciplinary University Research Initiative (MURI) project "Rapid Environmental Assessment Using an Integrated Coastal Ocean Observation-Modeling System (ESPRESSO)", and the Monterey Bay Aquarium Research Institute (MBARI). The objective of the NRL participation in the experiment was to study the variability and predictability of underwater light and coupled bio-optical and physical properties of the water column on time scales of 1 to 5 days.

2. SATELLITE MODIS-AQUA OCEAN COLOR DATA.

The MODIS-Aqua satellite imagery was processed using the NRL Automated Processing System (APS). APS is a complete end-to-end system that includes sensor calibration, atmospheric correction (with near-infrared correction for coastal waters), and bio-optical inversion. APS incorporates, and is consistent with, the latest NASA MODIS code (SeaDAS) (Gould et al., 2011, Martinolich and Scardino, 2011).

In this study, MODIS-Aqua chlorophyll-a (Chl) and absorption coefficient due to phytoplankton at 488 ($a_{ph}(488)$) data for June 5 and June 10 of 2008 are used for assimilation into the bio-optical, physical model. Chlorophyll data are derived by OC3M algorithm (O'Reilly et al., 2000), while $a_{ph}(488)$ data are derived by using a Quasi-Analytical Algorithm, QAA (Lee et al., 2002) at 1 km pixel resolution. Data are interpolated to the model grid spatially and temporally to 0Z and 12Z (with a12 hour data assimilation update cycle (see Data Assimilation section)).

3. COUPLED PHYSICAL, BIO-OPTICAL MODEL OF THE MONTEREY BAY.

The Monterey Bay model (called the NCOM ICON) consists of the physical model (Shulman et al., 2007), which is coupled to the biochemical model (Chai et al., 2002, Shulman et al., 2011). The physical model of the Monterey Bay is based on the NCOM model, which is a primitive-equation, 3D, hydrostatic model. It uses the Mellor-Yamada level 2.5 turbulence closure scheme, and the Smagorinsky formulation for horizontal mixing (Barron et al, 2006). The NCOM

ICON model is set up on a curvilinear orthogonal grid with resolution ranging from 1 to 4 km. The model is forced with surface fluxes from the Coupled Ocean and Atmospheric Mesoscale Prediction System (COAMPS®) (Doyle et al., 2009) at 3 km horizontal resolution. The 3-km resolution COAMPS® grid mesh is centered over Central California and the Monterey Bay. The biochemical model (the Carbon, Silicon, Nitrogen Ecosystem (CoSINE) model, Chai et al., 2002) of the NCOM ICON simulates the dynamics of two sizes of phytoplankton, small phytoplankton cells (< 5 μm in diameter) and diatoms, two zooplankton grazers, nitrate, silicate, ammonium, and two detritus pools. Constituents from the biochemical model are used to estimate chlorophyll and Inherent Optical Properties (IOPs) based on the methodology outlined by Fujii et al. (2007). Phytoplankton photosynthesis in the biochemical model is driven by Photosynthetically Active Radiation (PAR), which is estimated based on the shortwave radiation flux from the COAMPS® model. The Penta et al. (2008) scheme is used for PAR attenuation with depth. Open boundary conditions for the NCOM ICON are derived from the regional model of the California Current (NCOM CCS, Shulman et al., 2007). The NCOM CCS has a horizontal resolution of about 9 km and, the model is forced with atmospheric products derived from the COAMPS® (Doyle et al., 2009). As in NCOM ICON model, the biochemical model of the NCOM CCS is also 9-compartment model of Chai et al. (2002).

4. DATA ASSIMILATION.

For the assimilation of physical observations (temperature and salinity), the NCOM ICON model uses the Navy Coupled Ocean Data Assimilation (NCODA) system (Cummings, 2005, Cummings et al, 2009). The NCODA is a fully 3D multivariate optimum interpolation system. Assimilation of temperature and salinity data is performed every 12 hours (assimilation cycle). The NCODA assimilates satellite altimeter observations, satellite and in-situ sea surface temperature as well as available in-situ vertical temperature and salinity profiles from XBTs, ARGO floats, moored buoys and gliders from the Global Ocean Data Assimilation Experiment (GODAE) data set. The description of the data sets, processing and quality control procedures are described in (Cummings, 2006; Cummings et al., 2009). Results of glider, ship and satellite data assimilation into the NCOM ICON model are described in Shulman et al., 2009 and 2010. For assimilation of bio-optical properties a multivariate data assimilation approach (BOMA) has been developed. The analysis (updated) fields for the bio-optical model state variables are derived from:

$$\mathbf{X}^a = \mathbf{X}^f + \boldsymbol{K}(\mathbf{Y}^o - \boldsymbol{H}\mathbf{X}^f), \quad (1)$$

where $\mathbf{X}^a$ is vector of the analyzed bio-optical, physical properties, $\mathbf{X}^f$ is vector of the model forecast of bio-optical, physical properties, $\mathbf{Y}^o$ are available bio-optical, physical observations. $\boldsymbol{H}$ is the observational operator that maps the model state onto available observations, and $\boldsymbol{K}$ is the Kalman gain matrix, which depends on the forecast error covariance matrix $\boldsymbol{P}^f$ and the observation error covariance matrix, $\boldsymbol{R}$:

$$\boldsymbol{K} = \boldsymbol{P}^f \boldsymbol{H}^T (\boldsymbol{H}\boldsymbol{P}^f \boldsymbol{H}^T + \boldsymbol{R})^{-1}$$

In this study, (1) is used only to derive analyzed bio-optical state variables, because physical model state variables are updated by the NCODA system. Note, $\mathbf{Y}^o$ can contain not only bio-optical observations but also physical observations.

The multivariate forecast error covariance matrix $\boldsymbol{P}^f$ is estimated in the reduced EOF spectrum derived from the model run. In this study, we assimilated MODIS-Aqua derived chlorophyll and absorption coefficient due to phytoplankton at 488nm, described in Section 2.

5. DATA ASSIMILATION EXPERIMENTS DESIGN

Run 1 is the base run of the NCOM ICON model. The run was initialized from the NCOM CCS model on 22 May of 2008 and was run until the end of June without any assimilation of physical or bio-optical observations. The output from the Run 1 (during the month of June) is used to estimate error covariance $\boldsymbol{P}^f$ in Section 4. All runs described below started from the restart file from the Run 1 (physical and bio-optical state variables) on 5 June 00Z, and were run for 5 days until 10 June 00Z.

Run 2 is the run with the assimilation of only physical observations with a 12 hour data assimilation cycle. None of the bio-optical data listed in Section 2 were assimilated in Run 2. Comparisons of Run 2 with the base Run1 highlight the impact of just physical data assimilation on the model predictions of physical, as well as, bio-optical properties on time scales of 1 to 5 days.

Run 3 is the run with the assimilation of physical data as in the Run 2, but for each 12 hours, MODIS-Aqua Chl data (described in Section 2) are assimilated using BOMA (Section 4). In accord with (1), the only analyzed (updated) bio-optical properties were small phytoplankton ($\boldsymbol{P1}$) and diatoms ($\boldsymbol{P2}$). Therefore, for each 12 hours of the model

run, the NCODA assimilated physical observations and created a new restart file with updated (analyzed) temperature and salinity fields. Using this NCODA created restart file, the BOMA assimilated MODIS-Aqua Chl data and created a new restart file (nowcast) with updated (analyzed) $\boldsymbol{P1}$ and $\boldsymbol{P2}$. The next segment of the model run was started from this BOMA created restart file and was run for 12 hours until the next model restart file is created. Comparisons of Runs 3 and 1 show the impact of assimilations of physical, as well as MODIS-Aqua Chl data on the model predictions of bio-optical properties.

The Run 4 is a clone of Run 3, but the MODIS-Aqua phytoplankton absorption coefficient at 488nm ($\boldsymbol{a_{ph}(488)}$) data are assimilated in the model instead of the MODIS-Aqua Chl data as in Run 3. Comparisons of Runs 4 and 3 will provide the impact of the assimilation of surface absorption coefficient versus chlorophyll data on the model predictions of bio-optical properties on time scales 1 to 5 days.

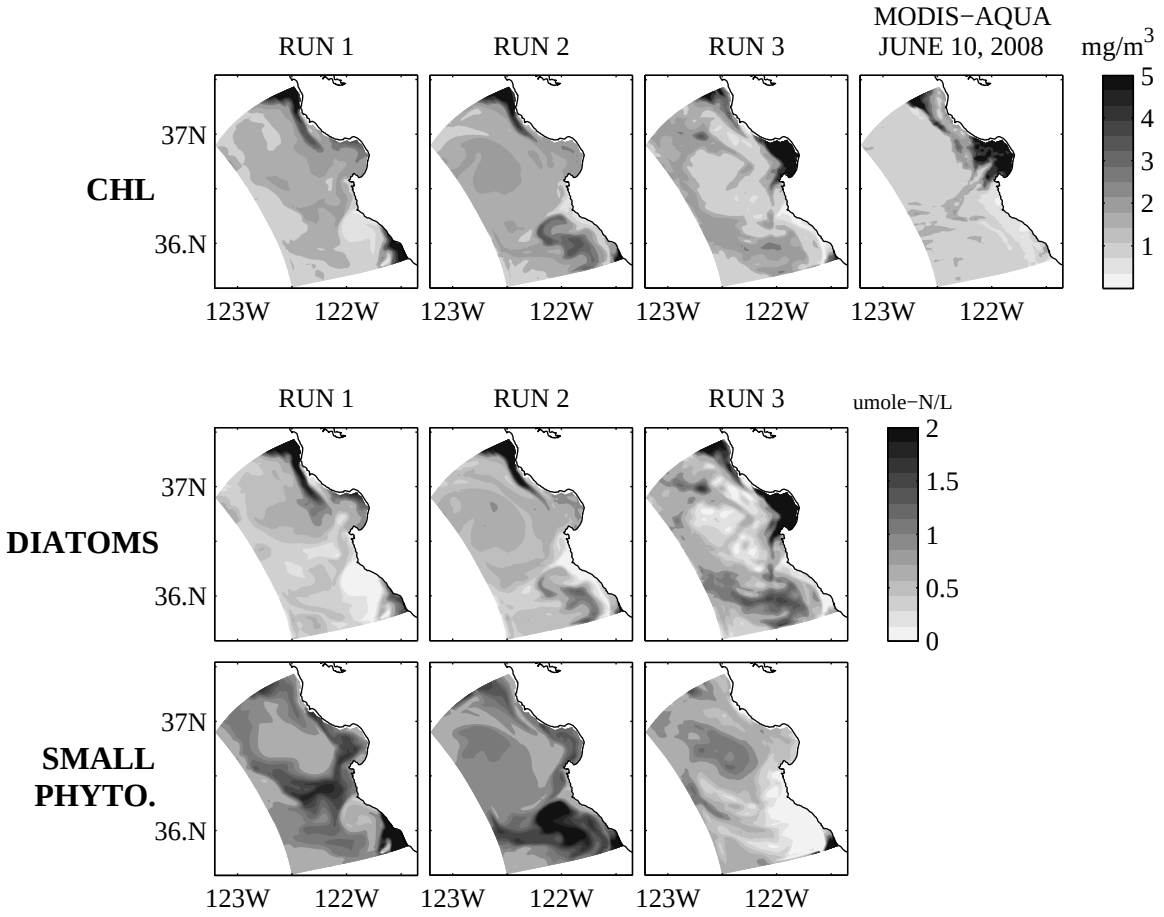

Figure 1. Observed MODIS-Aqua and model predicted chlorophyll and phytoplankton distributions on 10 June of 2010.

6. RESULTS

Figure 1 provides a comparison of surface chlorophyll properties for Runs 1, 2 and 3. Without the assimilation of MODIS-Aqua Chl , the model predicts lower chlorophyll values in the Bay for both cases of with (Run 2) or without (Run 1) assimilations of physical observations. In agreement with satellite observations, the assimilation of MODIS-Aqua Chl increased the model productivity inside the bay and decreased productivity outside the bay. Comparisons with the unassimilated Chl profiles from the water samples (Figure 2) demonstrate that the assimilation of surface MODIS-Aqua bio-optical products (surface Chl-a or $a_{ph}(488)$) improved not only surface, but also subsurface model chlorophyll predictions in the case of Runs 3 and 4 (in comparison to independent, not assimilated chlorophyll profiles from the water samples).

Quantitatively, this is also reflected in the Table 1, where RMSE between observed Chl-a from water samples and corresponding model-predicted Chl-a and $a_{ph}(488)$ values (at water samples locations) are presented. All RMSE metrics are normalized by the corresponding RMSE metric for the base Run 1 (no assimilation of physical as well as bio-optical properties).

Table 1. RMSE between observed and model-predicted chlorophyll distributions at water sample Sections A and B (Figure 2). RMSE are normalized by the RMSE for the base Run 1.

	SECT. A	SECT. B
RUN 1	1.00	1.00
RUN 2	1.01	1.02
RUN 3	0.71	0.95
RUN 4	0.65	0.83

Assimilation of MODIS-Aqua bio-optical observations increased (decreased) the concentration of diatoms (small phytoplankton) inside the Bay in comparison to non-assimilative RUNS 1 and 2 (Figure 1). This is well supported by comparisons of model predictions with observed fractions of microplankton (analog of diatoms in the model) versus total phytoplankton from the high performance liquid chromatography (HPLC) data presented on Figure 3. HPLC data indicate that there was steady presence of diatoms in the Bay between June 5 and 10, with the fraction of diatoms to total phytoplankton population in the range of 90 %. Runs 1 and 2 show variable fractions ranging from 20% to 80%, but mostly below the observed HPLC fractions. However, for Runs 3 (run with assimilation of MODIS-Aqua surface chlorophyll), the fraction of diatoms increased and partitioning between diatoms and small phytoplankton is in much better agreement with the independent, non assimilated HPLC observations. This is also reflected in the RMSE metrics presented in Table 2. With the assimilation of MODIS-Aqua Chl data, the RMS error between HPLC observed and model-predicted fractions of diatoms to the total phytoplankton is more than twice smaller for Run 3 in comparison to the RMS error for non-assimilative base Run 1. There are also improvements in fractions of diatoms to the total phytoplankton predictions for Run 4 (assimilation of $a_{ph}(488)$) after a couple days of assimilation (Figure 3 and Table 2).

Table 2. RMSE between HPLC fractions and model predicted fractions of diatoms to total phytoplankton population. RMSE are normalized by the RMSE for the base RUN 1.

	RMSE
RUN 1	1.00
RUN 2	0.92
RUN 3	0.43
RUN 4	0.84

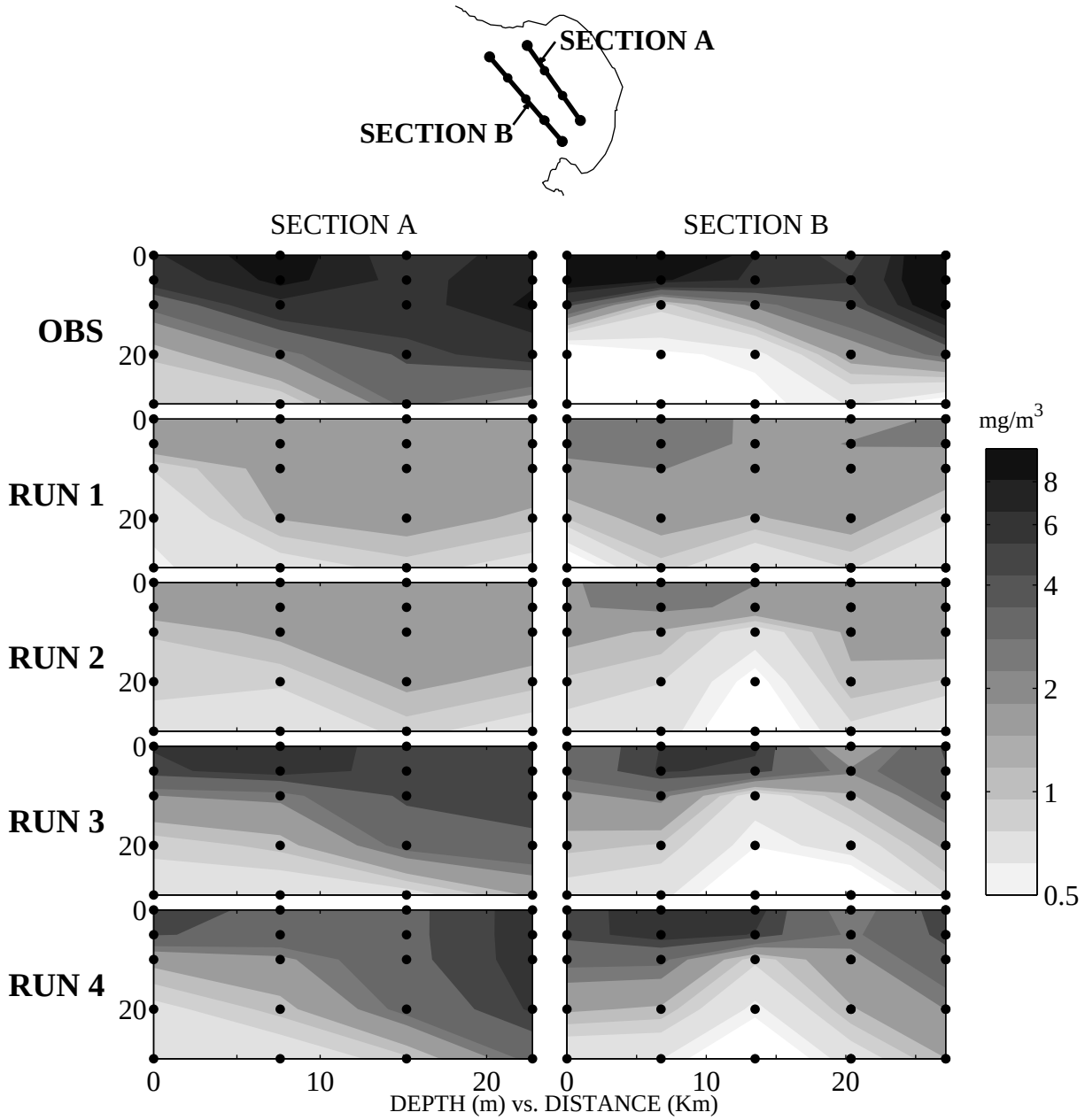

Figure 2. Comparisons of observed (Section A and B) and model-predicted subsurface chlorophyll distributions at water samples locations.

7. CONCLUSIONS AND DISCUSSIONS.

Data assimilation experiments were conducted during five days of steady upwelling in the Monterey Bay area. The results show that assimilation of MODIS-Aqua derived optical properties (chlorophyll or absorption due to

phytoplankton) significantly improved surface and subsurface agreement between the model and observations. Results show that the reduction in RMSE errors between model and independent water samples ranging from 5% to 35% in contrast to the non-assimilative run.

Assimilation of bio-optical data also improved fractionation of phytoplankton bio-mass between diatoms and small phytoplankton in the model. Without assimilation, the percentage of diatoms varied during the experiment between 20% and 80%. In contrast, HPLC measurements showed that the fraction of diatoms to total phytoplankton population in the range of 90%. However, runs with the assimilation of MODIS-Aqua surface chlorophyll produced much better agreement with the independent, non assimilated HPLC observations. With the assimilation, the RMSE error between HPLC observed and model-predicted fractions of diatoms to the total phytoplankton is less than half smaller the RMSE error for non-assimilative run. There are also improvements in fractions of diatoms to the total phytoplankton predictions for the run with assimilation of $\boldsymbol{a_{ph}(488)}$ after a couple days of assimilation.

In the present study, assimilation of physical properties through the NCODA and assimilation of bio-optical properties through BOMA are separated. The adjustment of updated physical and bio-optical variables is achieved through the coupled, bio-optical physical model run during the data assimilation cycle. At the same time, an instantaneous joint update of physical and bio-optical properties is preferred in order to maintain dynamical consistency between the assimilated physical and bio-optical fields. The merger of NCODA and BOMA is another topic of our future research.

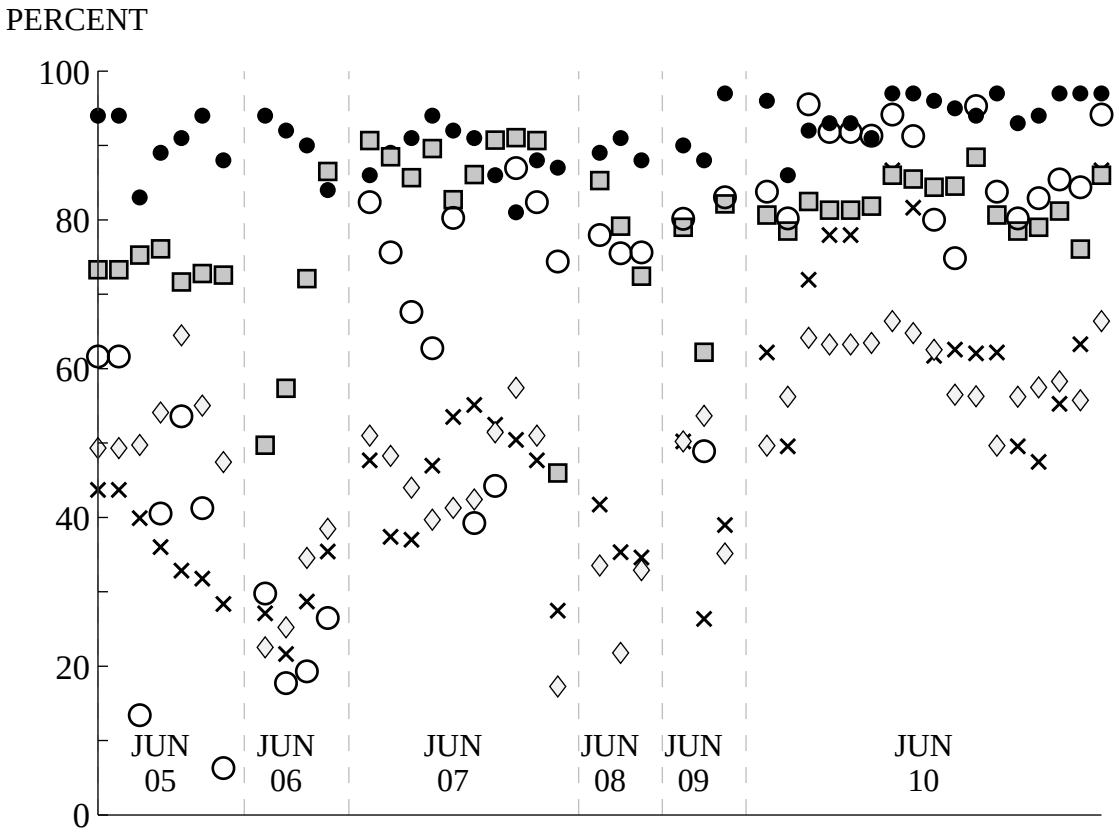

Figure 3. Observed and model-predicted fractions of diatoms to the whole phytoplankton populations at locations of water samples. Filled Circle- HPLC observed fractions; X- Run 1; Diamond – Run 2; Filled Square – Run 3 and Open Circle is Run 4.

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REFERENCE

Barron, C. N., A. B. Kara, P. J. Martin, R. C. Rhodes, and L. F. Smedstad, 2006: Formulation, implementation and examination of vertical coordinate choices in the global Navy Coastal Ocean Model (NCOM). Ocean Modelling, 11, 347–375, doi:10.1016/j.ocemod.2005.01.004.

Chai, F., R. C. Dugdale, T.-H. Peng, F. P. Wilkerson, and R. T. Barber (2002), One-dimensional ecosystem model of the equatorial Pacific upwelling system. Part I: Model development and silicon and nitrogen cycle, Deep Sea Res. Part II, 49, 2713–2745, doi:10.1016/S0967-0645 (02)00055-3.

Cummings, J., L. Bertino, P Brasseur, I. Fukumori, M. Kamachi, M. J. Martin, K. Mogensen, P. Oke, C. E. Testud, J. Verron, and A. Weaver, 2009: Ocean Data Assimilation Systems for GODAE, Oceanography, 22, 3, 96-109.

Cummings, J. A. (2005), Operational multivariate ocean data assimilation, Q. J. R. Meteorol. Soc., 131, 3583–3604, doi:10.1256/qj.05.105.

Doyle, J. D., Q. Jiang, Y. Chao, and J. Farrara (2009), high-resolution real-time modeling of the marine atmospheric boundary layer in support of the AOSN-II field campaign, Deep Sea Res. Part II, 56, 87–99.

Fujii, M., E. Boss, and F. Chai (2007), The value of adding optics to ecosystem models: A case study, Biogeosciences, 4, 817–835, doi:10.5194/bg-4-817-2007.

Gould, Jr., R.W., S.C. McCarthy, I. Shulman, E. Coelho, and J. Richman. 2011. Estimating Uncertainties in Bio-Optical Products Derived From Satellite Ocean Color Imagery Using an Ensemble Approach. Proc. of SPIE, Remote Sensing of the Ocean, Sea Ice, Coastal Waters, and Large Water Regions 2011, C.R. Bostater, Jr., S.P. Mertikas, Z. Neyt, and M. Velez-Reyes (eds.), Vol. 8175: 817506-01 – 817506-10. doi: 10.1117/12.897614.

Lee, Z, K. L. Carder, and R.A. Arnone, "Deriving inherent optical properties from water color: a multiband quasi-analytical algorithm for optically deep waters," Appl. Opt. 41, 5755-5772 (2002)

Martinolich, P. and Scardino, T., "Automated Processing System User's Guide Version 4.2," NRL, Washington, D.C., http://www7333.nrlssc.navy.mil/docs/aps_v4.2/html/user/aps_chunk/index.xhtml (2011).

O'Reilly, J. E., and 24 Coauthors, "SeaWiFS Postlaunch Calibration and Validation Analyses, Part 3," NASA Tech. Memo. 2000-206892, Vol. 11, S.B. Hooker and E.R. Firestone, Eds., NASA Goddard Space Flight Center, 49 pp. (2000).

Penta, B., Z. Lee, R. Kudela, S. Palacios, D. Gray, J. Jolliff, and I. Shulman (2008), An underwater light attenuation scheme for marine ecosystem models, Opt. Express, 16, 16,581–16,591.

Shulman, I., M. A. Moline, B. Penta, S. Anderson, M. Oliver, and S. H. D. Haddock (2011), Observed and modeled bio-optical, bioluminescent, and physical properties during a coastal upwelling event in Monterey Bay, California, J. Geophys. Res., 116, C01018, doi:10.1029/2010JC006525.

Shulman, I., S. Anderson, C. Rowley, S. deRada, J. Doyle, and S. Ramp (2010), Comparisons of upwelling and relaxation events in the Monterey Bay area, J. Geophys. Res., 115, C06016, doi:10.1029/2009JC005483.

Shulman, I., et al. (2009), Impact of glider data assimilation on the Monterey Bay model, Deep Sea Res. Part II, 56, 128–138.

Shulman, I., J. Kindle, P. Martin, S. deRada, J. Doyle, B. Penta, S. Anderson, F. Chavez, J. Paduan, and S. Ramp (2007), Modeling of upwelling/relaxation events with the Navy Coastal Ocean Model, J. Geophys. Res., 112, C06023, doi:10.1029/2006JC003946.